

Metal-insulator transition in a one-dimensional magnetic-non-magnetic superlattice geometry: Existence of multiple mobility edges

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Based on Green's function formalism, the existence of multiple mobility edges in a one-dimensional magnetic-non-magnetic superlattice geometry in presence of external electric field is predicted, and, it leads to the possibility of getting a metal-insulator transition at multiple values of Fermi energy. The role of electric field on electron localization is discussed for different arrangements of magnetic and non-magnetic atomic sites in the chain. We also analyze that the model quantum system can be used as a perfect spin filter for a wide range of energy.

PACS numbers: 73.63.Nm, 72.20.Ee, 73.21.-b, 73.63.Rt

I. INTRODUCTION

Quantum transport in low-dimensional systems has been a topic of interest within the past few decades due to its potential applicability in the field of nanoscience and nanotechnology. Exploitation of the spin degree of freedom adds a possibility of integrating memory and logic into a single device, leading to remarkable development in the fields on magnetic data storage application, device processing technique, quantum computation¹, etc. Naturally a lot of attention has been paid to study spin transport in low-dimensional systems both from experimental²⁻⁴ and theoretical⁵⁻¹⁵ points of view.

The understanding of electronic localization in low-dimensional model quantum systems is always an interesting issue. Whereas, it is a well established fact that in an infinite one-dimensional (1D) system with random site potentials all energy eigenstates are exponentially localized irrespective of the strength of randomness due to Anderson localization¹⁶, there exists another kind of localization, known as Wannier-Stark localization, which results from a static bias applied to a regular 1D lattice, even in absence of any disorder¹⁷. Till date a large number of works have been done to explore the understanding of Anderson localization and scaling hypothesis in one- and two-dimensional systems¹⁸. Similarly, Wannier-Stark localization has also drawn the attention of many theorists¹⁹⁻²³ as well as experimentalists²⁴. For both these two cases, viz, infinite 1D materials with random site energies and 1D systems subjected to an external electric field, one never encounters any *mobility edge* i.e., energy eigenvalues separating localized states from the extended ones, since all the eigenstates are localized. But there exist some special types of 1D materials, like quasi-periodic Aubry-Andre model and correlated disordered systems where mobility edge phenomenon at some particular energies is obtained²⁵⁻³⁴. Although the studies involving mobility edge phenomenon in low-dimensional systems have already generated a wealth of literature³²⁻³⁷ there is still need to look deeper into the problem to ad-

dress several interesting issues those have not yet been explored. For example, whether the mobility edges can be observed in some other simple 1D materials or the number of mobility edges separating the extended and localized regions in the full energy band of an 1D material can be regulated, are still to be investigated.

To address these issues in the present article we investigate two-terminal spin dependent transport in a 1D mesoscopic chain composed of magnetic and non-magnetic atomic sites in presence of external electric field. To the best of our knowledge, no rigorous effort has been made so far to explore the effect of an external electric field on electron transport in such a 1D magnetic-non-magnetic superlattice geometry. Here we show that, depending on the unit cell configuration, a 1D superlattice structure subjected to an external electric field exhibits multiple mobility edges at different values of the carrier energy. We use a simple tight-binding (TB) framework to illustrate the model quantum system and numerically evaluate two-terminal spin dependent transmission probabilities through the superlattice geometry based on the Green's function formalism. From our exact numerical analysis we establish that a sharp crossover from a completely opaque to a fully or partly transmitting zone takes place which leads to a possibility of tuning the electron transport by gating the transmission zone. In addition to this behavior we also show that the magnetic-non-magnetic superlattice structure can be used as a pure spin filter for a wide range of energy. These phenomena enhance the prospect of such simple superlattice structures as switching devices at multiple energies as well as spin filter devices, the design of which has significant impact in the present age of nanotechnology.

With an introduction in Section I, we organize the paper as follows. In Section II, first we present the model, then describe the theoretical formulation which include the Hamiltonian and the formulation for transmission probabilities through the model quantum system. The numerical results are illustrated in Section III and finally, in Section IV, we draw our conclusions.

II. THEORETICAL FRAMEWORK

Let us start with Fig. 1 where a 1D mesoscopic chain composed of magnetic and non-magnetic atomic sites is attached to two semi-infinite 1D non-magnetic electrodes, namely, source and drain. The chain consists of p (p being an integer) number of unit cells in which

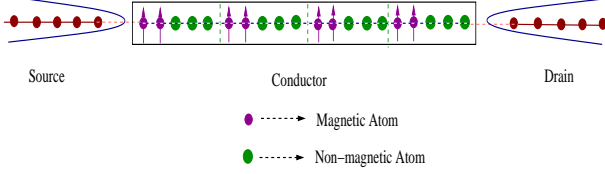


FIG. 1: (Color online). A 1D mesoscopic chain composed of magnetic (filled magenta circle) and non-magnetic (filled green circle) atomic sites is attached to two semi-infinite 1D non-magnetic metallic electrodes, namely, source and drain.

each unit cell contains n and m numbers of magnetic and non-magnetic atoms, respectively. Both the chain and side-attached electrodes are described by simple TB framework within nearest-neighbor hopping approximation.

The Hamiltonian for the entire system can be written as a sum of three terms as,

$$H = H_c + H_l + H_{tun}. \quad (1)$$

The first term represents the Hamiltonian for the chain and it reads

$$H_c = \sum_i c_i^\dagger (\epsilon_i + \vec{h}_i \cdot \vec{\sigma}) c_i + \sum_i [c_i^\dagger t c_{i+1} + h.c.] \quad (2)$$

where, $c_i^\dagger = \begin{pmatrix} c_{i\uparrow}^\dagger & c_{i\downarrow}^\dagger \end{pmatrix}$; $c_i = \begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix}$; $\epsilon_i = \begin{pmatrix} \epsilon_i & 0 \\ 0 & \epsilon_i \end{pmatrix}$;

$t = t \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$; and

$$\vec{h}_i \cdot \vec{\sigma} = h_i \begin{pmatrix} \cos \theta_i & \sin \theta_i e^{-j\phi_i} \\ \sin \theta_i e^{j\phi_i} & -\cos \theta_i \end{pmatrix}.$$

Here, ϵ_i refers to the on-site energy of an electron at the site i with spin σ (\uparrow, \downarrow), t is the nearest-neighbor hopping strength, $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) is the creation (annihilation) operator of an electron at the i th site with spin σ and h_i is the strength of local magnetic moment where $h_i = 0$ for non-magnetic sites. The term $\vec{h}_i \cdot \vec{\sigma}$ corresponds to the interaction of the spin of the injected electron with the local magnetic moment placed at the site i . The direction of magnetization in each magnetic site is chosen to be arbitrary and specified by angles θ_i and ϕ_i in spherical polar co-ordinate system for the i th atomic site. Here, θ_i represents the angle between the direction of magnetization and the chosen Z axis, and ϕ_i represents the azimuthal angle made by the projection of the local moment on X - Y plane with the X axis. In presence of bias voltage V between the source and

drain an electric field is developed, and therefore, the site energies of the chain becomes voltage dependent. Mathematically we can express it as $\epsilon_i = \epsilon_i^0 + \epsilon_i(V)$, where ϵ_i^0 is the voltage independent term. The voltage dependence of $\epsilon_i(V)$ reflects the bare electric field in the bias junction as well as screening due to longer range electron-electron interaction. In the absence of such screening the electric field varies uniformly along the chain and it reads $\epsilon_i(V) = V/2 - iV/(N+1)$, where N corresponds to the total number of atomic sites in the chain. In our present work, we consider both the linear and screened electric field profiles. As illustrative

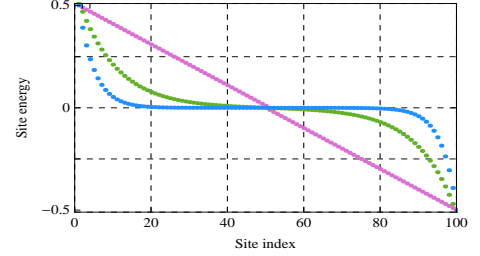


FIG. 2: (Color online). Voltage dependent site energies in a 1D chain considering 100 atomic sites for three different electrostatic potential profiles when the bias voltage V is set equal to 1.

example, in Fig. 2 we show the variation of voltage dependent site energies for three different electrostatic potential profiles for a chain considering 100 atomic sites and describe the nature of electronic localization for these profiles in the forthcoming section.

The second and third terms of Eq. 1 describe the TB Hamiltonians for the 1D semi-infinite non-magnetic electrodes and the chain-to-electrode coupling. These Hamiltonians are written as follows.

$$H_l = \sum_{\alpha=S,D} \left[\sum_n c_n^\dagger \epsilon_l c_n + \sum_n [c_n^\dagger t_l c_{n+1} + h.c.] \right] \quad (3)$$

and,

$$\begin{aligned} H_{tun} &= H_{tun,S} + H_{tun,D} \\ &= \tau_s [c_1^\dagger c_0 + h.c.] + \tau_d [c_N^\dagger c_{N+1} + h.c.]. \end{aligned} \quad (4)$$

The summation over S and D in Eq. 3 implies the incorporation of both the two electrodes, viz, source and drain. ϵ_l and t_l stand for the site energy and nearest-neighbor coupling, respectively. The electrodes are directly coupled to the chain through the lattice sites 1 and N , and the coupling strengths between these electrodes with the chain are described by τ_s and τ_d , respectively.

To obtain spin resolved transmission probabilities of an electron through the source-chain-drain bridge system, we use Green's function formalism. The single particle Green's function operator representing the entire system for an electron with energy E is defined as,

$$G = (E - H + i\eta)^{-1} \quad (5)$$

where, $\eta \rightarrow 0^+$.

Following the matrix form of \mathbf{H} and \mathbf{G} the problem of finding \mathbf{G} in the full Hilbert space \mathbf{H} can be mapped exactly to a Green's function \mathbf{G}_c^{eff} corresponding to an effective Hamiltonian in the reduced Hilbert space of the chain itself and we have,

$$\mathcal{G} = \mathbf{G}_c^{eff} = \sum_{\sigma} (\mathbf{E} - \mathbf{H}_c - \Sigma_S^{\sigma} - \Sigma_D^{\sigma})^{-1}, \quad (6)$$

where,

$$\Sigma_{S(D)}^{\sigma} = \mathbf{H}_{tun,S(D)}^{\dagger} \mathbf{G}_{S(D)} \mathbf{H}_{tun,S(D)}. \quad (7)$$

These Σ_S and Σ_D are the self-energies introduced to incorporate the effect of coupling of the chain to the source and drain, respectively. Using Dyson equation the analytic form of the self energies can be evaluated as follows,

$$\Sigma_{S(D)}^{\sigma} = \frac{\tau_{s(d)}^2}{E - \epsilon_l - \xi_l} \quad (8)$$

where, $\xi_l = (E - \epsilon_l)/2 - i\sqrt{t_l^2 - (E - \epsilon_l)^2/4}$.

Following Fisher-Lee relation, the transmission probability of an electron from the source to drain is given by the expression,

$$T_{\sigma\sigma'} = \text{Tr}[\mathbf{\Gamma}_S^{\sigma} \mathcal{G}^r \mathbf{\Gamma}_D^{\sigma'} \mathcal{G}^a]. \quad (9)$$

where, $\mathbf{\Gamma}_{S(D)}^{\sigma}$'s are the coupling matrices representing the coupling between the chain and the electrodes and they are defined as,

$$\mathbf{\Gamma}_{S(D)}^{\sigma} = i \left[\Sigma_{S(D)}^{\sigma} - \Sigma_{S(D)}^{\sigma\dagger} \right]. \quad (10)$$

Here, Σ_k^{σ} and $\Sigma_k^{\sigma\dagger}$ are the retarded and advanced self-energies associated with the k -th ($k = S, D$) electrode, respectively.

Finally, we determine the average density of states (ADOS), $\rho(E)$, from the following relation,

$$\rho(E) = -\frac{1}{N\pi} \text{Im} [\text{Tr}[\mathcal{G}]]. \quad (11)$$

In what follows we limit ourselves to absolute zero temperature and use the units where $c = e = h = 1$. For the numerical calculations we set $t = 1$, $\epsilon_i^0 = 0 \forall i$, $h_i = 1$ for the magnetic sites, $\theta_i = \phi_i = 0$, $\epsilon_l = 0$, $t_l = 1$ and $\tau_s = \tau_d = 0.8$. The energy scale is measured in unit of t .

III. NUMERICAL RESULTS AND DISCUSSION

Throughout our numerical calculations we assume that the magnetic moments are aligned along $+Z$ direction ($\theta_i = \phi_i = 0$), which yields vanishing spin flip transmission probability, viz, $T_{\uparrow\downarrow} = T_{\downarrow\uparrow} = 0$, across the bridge system. The net transmission probability is therefore a sum $T(E) = T_{\uparrow\uparrow}(E) + T_{\downarrow\downarrow}(E)$, and the origin of this zero spin

flipping can be explained from the following arguments. The operators $\sigma_+ (= \sigma_x + i\sigma_y)$ and $\sigma_- (= \sigma_x - i\sigma_y)$ associated with the term $\tilde{\mathbf{h}}_i \cdot \tilde{\boldsymbol{\sigma}}$ in the TB Hamiltonian Eq. 2 are responsible for the spin flipping, where $\tilde{\boldsymbol{\sigma}}$ being the Pauli spin vector with components σ_x , σ_y and σ_z for the injecting electron. In our present model since we consider that all the magnetic moments are aligned along $+Z$ direction, the term $\tilde{\mathbf{h}}_i \cdot \tilde{\boldsymbol{\sigma}} (= h_{ix}\sigma_x + h_{iy}\sigma_y + h_{iz}\sigma_z)$ gets the form $h_{iz}\sigma_z$, and accordingly, the Hamiltonian does not contain σ_x and σ_y and so σ_+ and σ_- do not appear,

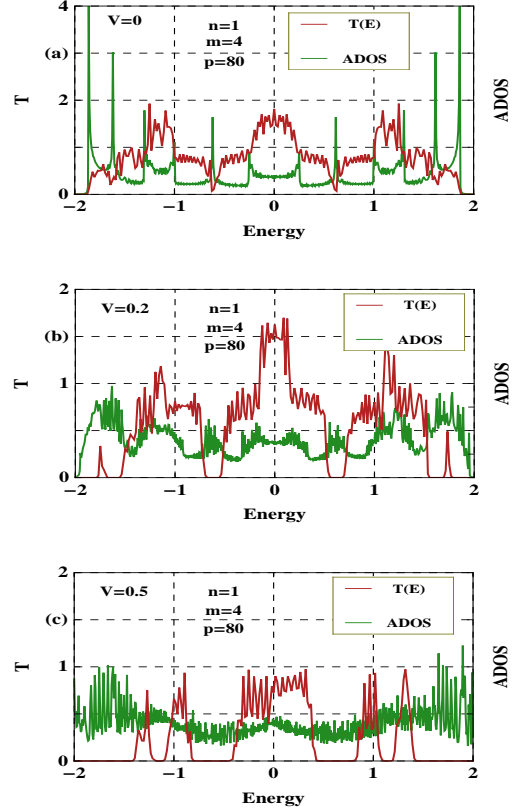


FIG. 3: (Color online). Transmission probability T and ADOS as a function of energy for a 1D magnetic-non-magnetic superlattice geometry considering a linear bias drop along the chain, as shown by the pink curve in Fig. 2, where (a)-(c) correspond to the results for three different values of bias voltage V .

which leads to the vanishing spin flip transmission probability across the 1D chain. Below, we address the central results of our study i.e, the possibility of getting multiple mobility edges in 1D magnetic-non-magnetic superlattice geometries and how such a simple model quantum system can be used as a perfect spin filter for a wide range of energy.

In Fig. 3 we show the variation of total transmission probability T along with the average density of states for a 1D magnetic-non-magnetic superlattice geometry considering a linear bias drop. Here we consider a 400-site chain in which each unit cell contains one magnetic

and four non-magnetic sites and the results are shown for three different bias voltages. For the particular case when the chain is free from external electric field i.e., $V = 0$ electronic conduction through the bridge takes place for the entire energy band as shown in Fig. 3(a) which predicts that all the energy eigenstates are extended in nature. The situation becomes really very interesting when the superlattice geometry is subjected to an external electric field. It is illustrated in Figs. 3(b) and 3(c). From

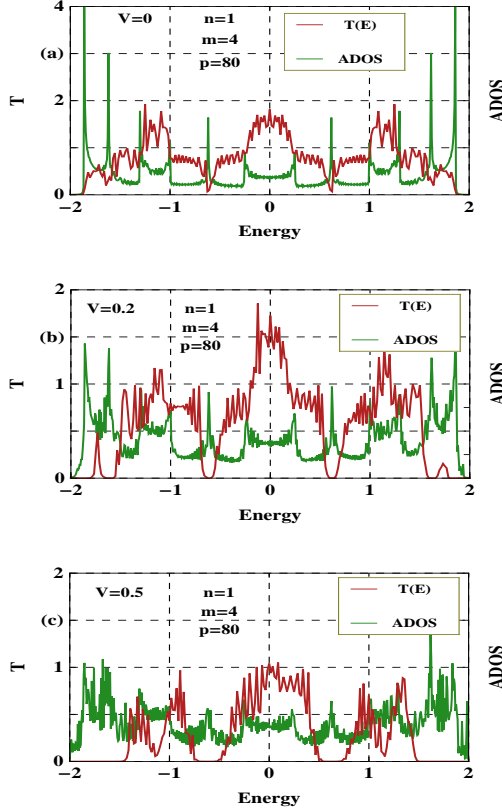


FIG. 4: (Color online). Transmission probability T and ADOS as a function of energy for a 1D magnetic-non-magnetic superlattice geometry when the electrostatic potential profile varies following the green curve shown in Fig. 2, where (a)-(c) represent the identical meaning as in Fig. 3.

these spectra we notice that there are some energy regions for which the transmission probability completely drops to zero which reveals that the eigenstates associated with these energies are localized, and they are separated from the extended energy eigenstates. Thus, sharp mobility edges are obtained in the spectrum, and, the total number of such mobility edges separating the extended and localized regions in a superlattice geometry in presence electric field strongly depends on the unit cell configuration and it can be regulated by adjusting the number of magnetic and non-magnetic sites. This phenomenon describes the existence of multiple mobility edges in a superlattice geometry under finite bias condition. Now if the Fermi energy is fixed at a suitable

energy zone where T drops to zero an insulating phase will appear, while for the other case, where T is finite, a metallic phase is observed and it leads to the possibility of controlling the electronic transmission by gating the transmission zone. The width of the localized regions between the band of extended regions increases with the strength of the electric field as clearly shown by com-

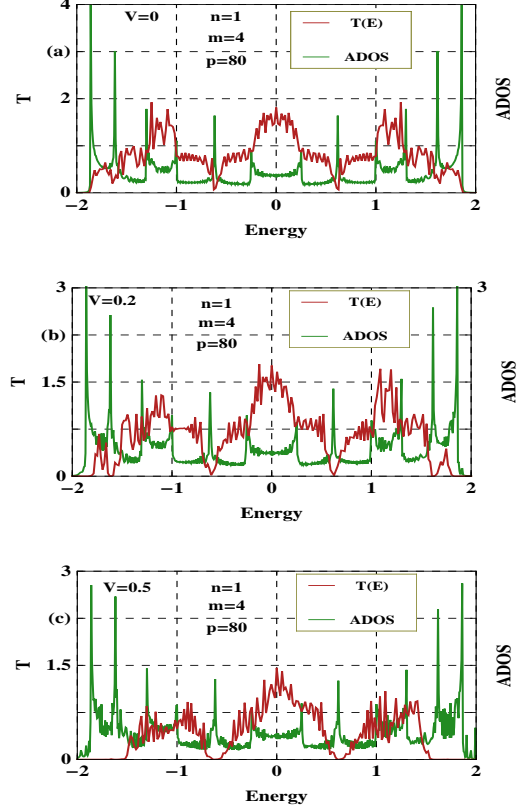


FIG. 5: (Color online). Transmission probability T and ADOS as a function of energy for a 1D magnetic-non-magnetic superlattice geometry when the electrostatic potential profile varies following the blue curve shown in Fig. 2, where (a)-(c) represent the identical meaning as in Fig. 3.

paring the spectra given in Figs. 3(b) and 3(c), and, for strong enough field strength almost all energy eigenstates are localized. In that particular limit metal-to-insulator transition will no longer be observed.

The above results are analyzed for a particular (linear) variation of electric field along the chain. To explore the sensitivity of getting metal-to-insulator transition on the distribution of electric field, in Figs. 4 and 5 we present the results for two different screened electric field profiles taking the identical chain length. From the spectra we clearly observe that the width of the localized region gradually disappears with the flatness of the electric field profile in the interior of the bridge system. If the potential drop takes place only at the chain-to-electrode interfaces, i.e., when the potential profile becomes almost flat along the chain the width of the localized region almost

vanishes and the metal-to-insulator transition is not observed, as is the case for the zero bias limit.

Finally, we illustrate how such a simple magnetic-non-magnetic superlattice geometry can be utilized as a perfect spin filter for a wide range of energy in absence of any

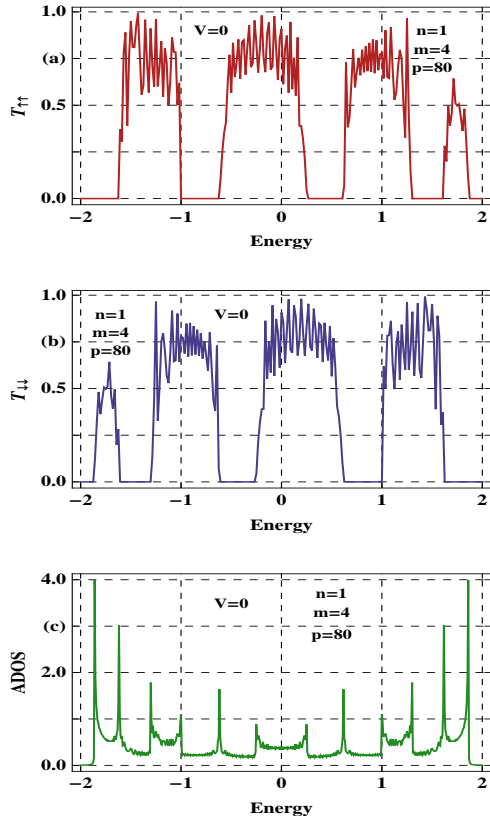


FIG. 6: (Color online). $T_{\uparrow\uparrow}$, $T_{\downarrow\downarrow}$ and ADOS as a function of energy for a 1D magnetic-non-magnetic superlattice geometry in absence of external electric field.

external electric field. As illustrative example, in Fig. 6 we present the transmission probabilities for up and down spin electrons together with the average density of states as a function of energy for a 1D magnetic-non-magnetic superlattice geometry. From the spectra we observe that the up and down spin electrons follow two different channels while traversing through the superlattice geometry, since the spin flipping is completely blocked for this configuration. This splitting of up and down spin conduction channels is responsible for spin filtering action and the total number of these channels strongly depends on the unit cell configuration. From Figs. 6(a) and (b) we clearly see that for a wide range of energy for which

the transmission probability of up spin electrons drops to zero value, shows non-zero transmission probability of down spin electrons. Therefore, setting the Fermi energy to a suitable energy region we can control the transmission characteristics of up and down spin electrons, and, a spin selective transmission is thus obtained through the bridge system. Before we end, we would like to point out that since the overlap between the up and down spin conduction channels depends on the magnitudes of the local magnetic moments, we can regulate the spin degree of polarization (DOP) simply by tuning the strength of these magnetic moments and for a wide range of energies it (DOP) almost reaches to 100%. Thus, our proposed magnetic-non-magnetic superlattice geometry is a very good example for designing a spin filter.

A. Conclusion

To conclude, in the present work we investigate in detail the spin dependent transport under finite bias condition through a 1D magnetic-non-magnetic superlattice geometry using Green's function formalism. We use a simple TB framework to describe the model quantum system where all the calculations are done numerically. From our exact numerical analysis we predict that in such a simple 1D magnetic-non-magnetic superlattice geometry multiple mobility edges separating the localized and extended regions are obtained in presence of external electric field and the total number of mobility edges in the full energy spectrum can be controlled by arranging the unit cell configuration. This phenomenon reveals that the superlattice geometry can be used as a switching device for multiple values of Fermi energy. The sensitivity of metal-to-insulator transition and vice versa on the electrostatic potential profile is thoroughly discussed. Finally, we analyze how such a superlattice geometry can be utilized in designing a tailor made spin filter device for wide range of energies. Setting the Fermi energy at a suitable energy zone, a spin selective transmission is obtained through the bridge system. All these predicted results may be utilized in fabricating spin based nano electronic devices.

The results presented in this communication are worked out for absolute zero temperature. However, they should remain valid even in a certain range of finite temperatures (~ 300 K). This is because the broadening of the energy levels of the chain due to the chain-to-electrode coupling is, in general, much larger than that of the thermal broadening³⁸.

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